Slides, notes, and exercises at:
https://github.com/cheshyre/nptls-hf

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

The Hartree-Fock method / Preparation for Python exercises

Nuclear Physics Turtle Lecture Series 2025:
Ab initio Hartree-Fock calculations of nuclei

Lecture 3

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Recap

- We have some V_{NN}, V_{3N}
- We have the relevant one-, two-, and three-body matrix elements of our kinetic energy T and our interactions V_{NN}, V_{3N}
- We want to construct our many-body Hamiltonian H
- And we want to solve the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$

- **This lecture:** Finding the best Slater determinant approximation to $|\Psi\rangle$

Main messages

- Ground state $|\Psi\rangle$ has minimum energy E_{gs} of any A-particle state
- Hartree-Fock state $|\Phi_{\mathrm{HF}}\rangle$ has min. energy $E_{\mathrm{gs}}^{\mathrm{HF}}$ of any Slater determinant
- Need to find **best basis** $|\bar{p}\rangle$ to construct $|\Phi_{\mathrm{HF}}\rangle$
- Intuitively, HF ...
  - ... identifies **average potential** felt by particles (with interactions)
  - ... **solves for eigenbasis** of this average potential → HF basis $|\bar{p}\rangle$

Hartree-Fock approximation on whiteboard

Intro to Python exercises on screen

Summary

- Fock matrix F is **average potential** felt by all particles
- **Diagonalizing Fock matrix** gives "best basis" (lowest energy state $|\Phi\rangle$)
- Key steps:
  - Build 1-body density matrix ρ_{pq} for current state $|\Phi_{\text{trial}}\rangle$
  - Compute Fock matrix F_{pq} based on ρ_{pq}
  - Diagonalize Fock matrix and get new state $|\Phi_{\text{trial}}\rangle$
  - The energy $\langle\Phi_{\text{trial}}|H|\Phi_{\text{trial}}\rangle$ decreases until we reach minimum E_{HF}